Optical pulse propagation in the tight-binding approximation

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Abstract: We formulate the equations describing pulse propagation in a one-dimensional optical structure described by the tight binding approximation, commonly used in solid-state physics to describe electrons levels in a periodic potential. The analysis is carried out in a way that highlights the correspondence with the analysis of pulse propagation in a conventional waveguide. Explicit expressions for the pulse in the waveguide are derived and discussed in the context of the sampling theorems of finite-energy space and time signals.

References and links

1. A. Yariv, *Optical Electronics in Modern Communications*, (Oxford University Press, 1997).
2. N.W. Ashcroft and N.D. Mermin, *Solid State Physics*, (Harcourt, 1976).
3. A. Yariv, Y. Xu, R.K. Lee, and A. Scherer, "Coupled-resonator optical waveguide: a proposal and analysis," Opt. Lett. **24**, 711 (1999).
4. Y. Xu, R.K. Lee, and A. Yariv, "Propagation and second-harmonic generation of electromagnetic waves in a coupled-resonator optical waveguide," J. Opt. Soc. Am. B **17** 387 (2000).
5. S. Mookherjea and A. Yariv, "Optical pulse propagation and holographic storage in a coupled-resonator optical waveguide," Submitted to Phys. Rev. E (June 2001).
6. M. Bayindir, B. Temelkuran, and E. Ozbay, "Tight-binding description of the coupled defect modes in three-dimensional photonic crystals," Phys. Rev. Lett. **84** 2140 (2000).
7. N.G.R. Broderick and C.M. de Sterke, "Theory of grating superstructures," Phys. Rev. E **55** 3634 (1997).
8. C.M. de Sterke, "Superstructure gratings in the tight-binding approximation," Phys. Rev. E **57** 3502 (1998).
9. J.D. Jackson, *Classical Electrodynamics*, third edition, (John Wiley & Sons, 1999).
10. T.M. Apostol, *Mathematical Analysis*, (Addison-Wesley, 1964).
11. A.V. Oppenheim, A.S. Willksy, and I.T. Young, *Signals and Systems*, (Prentice-Hall, 1995).
12. J.M. Wozencraft and I.M. Jacobs, *Principles of Communication Engineering*, (John Wiley & Sons, 1965).

1   Introduction

The application of coupled-mode theory to the problem of propagation in an optical waveguide is well known [1], and is particularly useful in the description of gratings and other periodic optical systems where the strength of the perturbation (relative to the free-space equations) is weak. Not surprisingly, the same formalism has been applied in solid state physics to the description of electrons in a weak periodic potential [2]. Complementary to this weakly perturbative approach is the tight binding approxmation, also known as the linear combination of atomic orbitals (LCAO), which describes electrons in a crystalline solid with a strong periodic potential due to the lattice structure

of localized atoms, characterized by a weak overlap between the atomic wave functions. By analogy, the optical structures that can be described using the tight binding approximation are those that consist of isolated structural elements (e.g., high-Q resonators such as defect modes in photonic crystals) weakly coupled to one another; the propagating eigenmodes of the overall system are then closely related to the eigenmodes of the individual elements, rather than the free-space eigenmodes as in coupled-mode theory.

We mention two applications of this description. Recently, a new type of waveguide based on the coupling of optical resonators has been introduced, called the Coupled Resonator Optical Waveguide (CROW) [3]. A weakly-coupled CROW is characterized a nearly flat dispersion relationship and potentially very low group velocity in the waveguide, which can be used for efficient second-harmonic generation [4] and, if designed e.g., in a photorefractive photonic crystal, for photorefractive holography of optical pulses leading to the possibility of optical pulse storage [5]. Recent experiments in the microwave regime have demonstrated the validity of the tight binding approximation in such a structure [6]. Another application of this framework is in the description of superstructure Bragg gratings (SSGs), also called optical superlattices, which are fiber or semiconductor gratings with parameters that vary periodically as a function of position [7]. Whereas shallow SSGs can be described by the standard coupled-mode theory, deep SSGs require the complementary approach of the tight-binding approximation [8].

In both these physical realizations of the tight binding approximation, the analysis has so far been restricted to the propagation of monochromatic waves at the eigenfrequencies of the structure. In this paper, we describe the propagation of pulses with a nonzero spread of wave vectors in a one-dimensional structure described by the tight binding approximation and comment on certain limits in which a simplified analysis is justifiable.

2 Eigenmodes in the tight-binding approximation

We assume that the structural elements comprising the periodic waveguide e.g., defect modes in a photonic crystal or photonic wells in the description of SSGs, are identical and lie along the z axis separated by a distance R. The total length of the device is taken to be L so that the number of elements is $N = L/R$. As indicated by the nomenclature "linear combination of atomic orbitals," the eigenmode of the time-independent Hamiltonian $\phi_k(z)$ at a particular wave vector k is written as a linear combination of the individual modes $\psi_l(z)$ of the elements that comprise the structure [2],

$$\phi_k(z) = \sum_n \exp(-inkR) \sum_l b_l\, \psi_l(z - nR) \tag{1}$$

where the summation over n runs over the N structural elements and the summation over l refers to the bound states in each individual element. In a CROW, for instance, the individual resonator modes are doubly degenerate [4], so that $l = \pm 1$, whereas in an SSG, it is usually sufficient to consider a single l [8]. We will assume that $\sum_l |b_l|^2 = 1$.

In the description of a structure of finite length, the wave vector k is restricted according to the Born-von Karman periodic boundary condition [2]

$$k_m = m\left(\frac{2\pi}{L}\right) \tag{2}$$

where m is an integer; k_m then ranges over the Brillouin zones and because $\phi_k(z)$ is of the Bloch form [2], we may only consider the first Brillouin zone $m = 0, 1, \ldots, N - 1$ to characterize the dispersion relationship in the structure [3]. From Eq. (2), $\Delta k \equiv k_{m+1} - k_m = 2\pi/L$ so that in the theoretical limit of an infinitely long structure, the discrete distribution of eigenmodes goes over to a continuous spectrum.

3   Pulse propagation in the tight-binding approximation

Assume that at time $t = 0$, the field in a structure of infinite length is given by a superposition of eigenmodes,

$$\mathcal{E}(z, t = 0) = \int \frac{dk}{2\pi} c_k \phi_k(z) \tag{3}$$

where $\phi_k(z)$ are the eigenmodes at wave vector k as given by Eq. (1) and c_k are certain 'weights' to be determined from the boundary condition.

For a structure of finite length, not all k vectors are allowed, according to Eq. (2), and the integral over k in Eq. (3) should be replaced by a sum over the allowed k. Alternatively, we can redefine $\phi_k(z)$ for a structure of finite length as

$$\phi_k(z) = \left[|\Delta k| \sum_{m=-\infty}^{\infty} \delta(k - m\Delta k) \right] \sum_n \exp(-inkR) \sum_l b_l \, \psi_l(z - nR) \tag{4}$$

to preserve the form of Eq. (3). The factor $|\Delta k|$ inside the square brackets in Eq. (4) follows from the usual definition of the Riemann-Stieltjes integral [10]: for an infinitely long structure, as $L \to \infty$ and $\Delta k \to 0$, the field $\mathcal{E}(z, t = 0)$ retains the form of Eq. (3) with $\phi_k(z)$ defined by Eq. (1), i.e., without the impulse train (in square brackets) in Eq. (4). In other words, we have defined the eigenmodes differently for the case of a finite length and infinite length so that the form of Eq. (3) is unchanged.

The system is linear and time invariant and therefore the field at time t is given by

$$\mathcal{E}(z, t) = \int \frac{dk}{2\pi} e^{i\omega(k)t} c_k \phi_k(z). \tag{5}$$

Since the dispersion relationships of the waveguide modes are approximately linear in the middle of the band gap (the group velocity goes to zero at the band edges) [3, 8], we can write the dispersion relationship around the central wave vector of the pulse k_0 as

$$\omega(k_0 + K) = \omega(k_0) + \left. \frac{d\omega}{dk} \right|_{k=k_0} K + \ldots \approx \omega_0 + v_g K \tag{6}$$

where v_g is the group velocity of the pulse. Then,

$$\mathcal{E}(z, t) = e^{i\omega_0 t} \int \frac{dK}{2\pi} e^{iv_g tK} c_{k_0+K} \, \phi_{k_0+K}(z). \tag{7}$$

The boundary conditions specify a pulse shape at the $z = 0$ edge of the waveguide and centered at the optical frequency ω_0,

$$\mathcal{E}(z = 0, t) = e^{i\omega_0 t} E(z = 0, t), \tag{8}$$

so that from the equality of Eq. (7) evaluated at $z = 0$ and Eq. (8), it follows that

$$c_{k_0+K} = \frac{1}{\phi_{k_0+K}(0)} \int d(|v_g|t') \, E(z = 0, t') e^{-iv_g t'K}. \tag{9}$$

Combining Eq. (7) and Eq. (9),

$$\mathcal{E}(z, t) = e^{i\omega_0 t} \int d(|v_g|t') \, E(z = 0, t') \int \frac{dK}{2\pi} \frac{\phi_{k_0+K}(z)}{\phi_{k_0+K}(0)} e^{iv_g(t-t')K}. \tag{10}$$

4 Free space propagation

In free space, which can be thought of as a 'linear space-invariant system,' the eigenfunctions are $\phi_k(z) = \exp(-ikz)$. Substituting this into Eq. (10), we get

$$
\begin{aligned}
\mathcal{E}(z,t) &= e^{i\omega_0 t} \int d(|v_g|t')\, E(z=0,t') \int \frac{dK}{2\pi}\, e^{-i(k_0+K)z}\, e^{iv_g(t-t')K} \\
&= e^{i(\omega_0 t - k_0 z)} E\left(z=0, t - \frac{z}{v_g}\right).
\end{aligned} \tag{11}
$$

This is the well-known result (similar to Jackson [9, pp. 322–326]) that a pulse propagates unchanged in shape in a weakly-dispersive medium, apart from an overall phase factor, and that the velocity of propagation is given by the group velocity of the pulse v_g defined from the dispersion relationship as in Eq. (6).

5 Simplifications

For a structure whose eigenmodes are given by Eq. (1) or Eq. (4) with $\psi(z)$ rapidly decaying in magnitude for distances on the order of R, we can carry out further simplifications to the field expression Eq. (10).

The individual resonator eigenmodes are normalized as $\psi_l(0) = 1$ and are highly localized around $z = 0$ so that $|\psi_l(nR)| \ll 1$ for all $n \neq 0$. We assume that these eigenmodes are symmetric, so that $\psi_l(-z) = \psi_l(z)$. Then,

$$
\begin{aligned}
\phi_{k_0+K}(0) &= \sum_n e^{-i(k_0+K)nR} \sum_l b_l\, \psi(-nR) \\
&= 1 + \sum_l b_l\, \psi_l(R)\, 2\cos[(k_0+K)R] + \dots
\end{aligned} \tag{12}
$$

ignoring terms on the order of $\sum_l b_l\, \psi(2R)$ or smaller. (The assumption of symmetry is only for convenience—the terms $n = -1$ and $n = 1$ can be considered separately.) Consequently, we can write

$$
[\phi_{k_0+K}(0)]^{-1} \approx 1 - \sum_l b_l\, \psi_l(R)\, 2\cos[(k_0+K)R], \tag{13}
$$

which can be used in Eq. (10).

The leading order contribution to $\mathcal{E}(z,t)$ follows from the first term of Eq. (13),

$$
\begin{aligned}
\mathcal{E}(z,t) &= e^{i\omega_0 t} \sum_n e^{-ik_0 nR} \sum_l b_l\, \psi_l(z-nR) \int d(|v_g|t')\, E(z=0,t') \\
&\quad \times \int \frac{dK}{2\pi} \left[|\Delta K| \sum_m \delta(K - m\Delta K) \right] e^{iTK}
\end{aligned} \tag{14}
$$

where $T \equiv v_g(t - nR/v_g - t')$, and we recognize that $k = k_0 + K$ so that $\Delta k = \Delta K$ and the index m of the infinite summation can be translated as desired. The second integral of Eq. (14) is the inverse Fourier transform (evaluated at T) of an impulse train in the K domain, which evaluates to an impulse train in the T domain [11], written as the Fourier transform relationship

$$
|\Delta K| \sum_{m=-\infty}^{\infty} \delta(K - m\Delta K) \overset{\mathcal{FT}}{=\!=} \sum_{m=-\infty}^{\infty} \delta(T - m\Delta T) \tag{15}
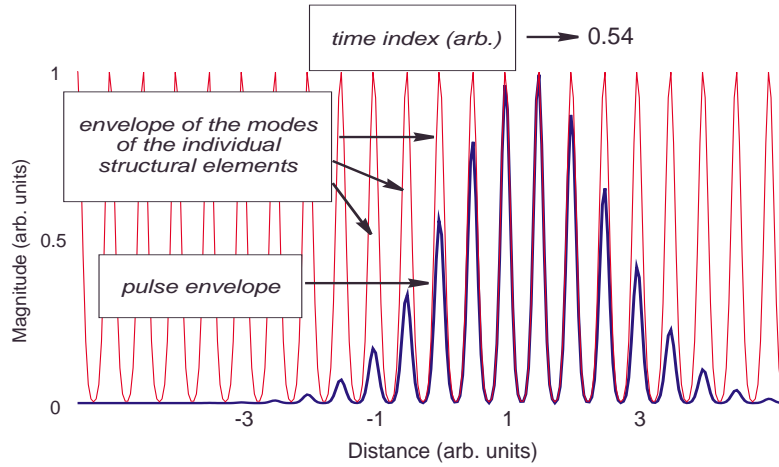$$

Fig. 1. (752 kB) Pulse propagation in a CROW structure described by the tight binding approximation. The envelope of the eigenmode of the structure is shown in red, and the Gaussian pulse envelope in blue, propagating from left to right, indexed by an arbitrary time coordinate at the upper-right corner.

where $\Delta T = 2\pi/\Delta K = L$. Carrying out the integrals over t' for each m,

$$\mathcal{E}(z,t) = e^{i\omega_0 t} \sum_n e^{-ik_0 nR} \sum_l b_l\, \psi_l(z - nR) \sum_m E\left(z = 0, t - \frac{nR + mL}{v_g}\right). \qquad (16)$$

This expression is the tight binding approximation analog of Eq. (11).

For individual resonator modes that are not quite so weakly confined, the contribution of the first-order corrections to Eq. (16) based on Eq. (13) can be evaluated in the same way,

$$
\begin{aligned}
\Delta\mathcal{E}(z,t) \;=\; & -\sum_{l'} b_{l'} \psi_{l'}(R) e^{i\omega_0 t} \Bigg\{ \sum_n e^{-ik_0(n-1)R} \sum_l b_l\, \psi_l(z - nR) \times \\
& \sum_m E\left(z = 0, t - \frac{(n-1)R + mL}{v_g}\right) + \sum_n e^{-ik_0(n+1)R} \times \\
& \sum_l b_l\, \psi_l(z - nR) \sum_m E\left(z = 0, t - \frac{(n+1)R + mL}{v_g}\right) \Bigg\}. \qquad (17)
\end{aligned}
$$

Fig. 1 shows an annotated frame from an MPEG animation of Gaussian pulse propagation in a structure described by the tight-binding approximation to the leading order, using the approximations that the structure is of infinite length and that it is sufficient to consider a single l in Eq. (16). For a structure of finite length with appropriate chosen pulses (as described in Section **6**), the results are exactly similar to the case shown above within the extent of the waveguide.

Although Eq. (7) is a good approximation to the dispersion relationship in a CROW [3, 4], it may be necessary for wideband pulses to consider higher-order terms in Eq. (7). The resulting Eq. (9) is then obtained from the solution of a Fredholm integral equation, and Eqs. (10) and (16) will in general involve envelope distortion (as for free space propagation [1].) Since this paper focuses on the general principles of undistorted pulse propagation in a CROW, this will be discussed elsewhere.

6 Frequency, space, and time sampling

As already noted, the allowed k vectors are quantized in a structure of finite length, and using Eq. (6), the allowed $\omega = \omega_0 + \Omega$ values are quantized. To prevent aliasing [11], ithe temporal interval between two samples $2\pi/\Delta\Omega$ must be greater than twice the temporal extent of the pulse envelope T, where $\Delta\Omega = v_g \Delta K$ according to Eq. (6)[1]. Therefore,

$$\frac{2\pi}{(2\pi/L)v_g} = 2T_{\max} \quad \text{which implies} \quad T_{\max} = \frac{1}{2}\frac{L}{v_g}. \tag{18}$$

In addition to the consequences of the dispersion relationship, the geometrical structure of the waveguide is also important. The eigenmode $\phi_k(z)$ represents a *spatial* sampling function for the propagating pulse envelope, especially in the limit that the individual strucural eigenmodes $\psi_l(z)$ are tightly confined (see Fig. 1). Again, to prevent aliasing, it is necessary that the spectral content in K-space be no greater than $K_{\max}$,

$$\frac{2\pi}{R} = 2K_{\max} \quad \text{which implies} \quad K_{\max} = \frac{1}{2}\left(\frac{2\pi}{R}\right). \tag{19}$$

But the free-space pulse envelope is invariant in the frame $z - v_g t$, and this maximum K-space extent translates into a *minimum* pulse width $T_{\min}$,

$$\frac{1}{2}v_g T_{\min} = R \quad \text{which implies} \quad T_{\min} = \frac{2R}{v_g}. \tag{20}$$

(As a guideline, it is useful to recall that the Fourier transform of a rectangular pulse between $\pm v_g T$ in the $v_g t$ frame is a *sinc* function with first nulls at $\pm \pi/(v_g T)$ in K-space [11]). In a structure of finite length described by the tight-binding approximation, therefore, there exists both a maximum and a minimum allowed pulse duration; the former arises because of the finite length of the structure, and the latter because of the sampling train-like eigenmodes of the waveguide.

Eq. (20) limits the bandwidth (where most of the energy of the pulse is concentrated) in the Fourier K-space associated with the propagation distance z, and since the pulse is propagating with group velocity v_g, also in the Fourier Ω-space associated with the temporal coordinate t. The dimension of the space of finite-energy signals (pulse envelopes) that are identically zero outside the time interval $[-T_0/2, T_0/2]$ and have most of their energy concentrated in the bandwidth $[-\Omega_0/2, \Omega_0/2]$ is approximately $D = \Omega_0 T_0 + 1$ [12],

$$D = \left(\frac{2\pi}{R}v_g\right)\left(\frac{1}{2}\frac{L}{v_g}\right) + 1 = \pi N + 1, \tag{21}$$

where $N = L/R$ is the number of individual structural elements in the waveguide. These pulse envelopes can be represented in the mean-square sense by a superposition of the prolate spheroidal wave functions within the interval $[-T_0/2, T_0/2]$.

Acknowledgments

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[1] A physical rationalization of this may be helpful: the spectrum of the field envelope in the waveguide is represented by a discrete set of complex exponentials with frequencies $\omega_0 + m\Delta\Omega$ according to Eq. (2) and the dispersion relationship, Eq. (6). To successfully characterize the continuous free-space spectral envelope by this discrete set, we require that within the time interval $T_{\max}$, the frequency change between succesive exponentials is "small," i.e., $T_{\max}\Delta\Omega < \pi$. The pulse envelope in the waveguide then consists of replicas of the free-space envelope, analogous to the spectral replicas formed by reconstruction of time-sampled signals [11].